Statistical approach of the modulational instability of the discrete self-trapping equation

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Abstract

The discrete self-trapping equation (DST) represents an useful model for several properties of one-dimensional nonlinear molecular crystals. The modulational instability of DST equation is discussed from a statistical point of view, considering the oscillator amplitude as a random variable. A kinetic equation for the two-point correlation function is written down, and its linear stability is studied. Both a Gaussian and a Lorentzian form for the initial unperturbed wave spectrum are discussed. Comparison with the continuum limit (NLS equation) is done.

1 Introduction

The discrete self-trapping (DST) equation

$$i\frac{da_n}{dt} - \omega_0 a_n + \lambda(a_{n+1} + a_{n-1}) + \mu|a_n|^2 a_n = 0 \tag{1}$$

is a typical equation for a system of harmonically coupled nonlinear oscillations [1], [2] relevant for several physical problems. We mention here only Davydov's model of energy transport in α-helix structures in proteins [3], [4], [2], where (1) appears as a certain approximation of the model. In (1) a_n is the complex classical dimensionless amplitude of the oscillator of frequency ω_0 in the n-th molecule, and λ, μ (of dimension of frequency) are the coupling constants between nearest neighbour oscillators and the one-site nonlinearity respectively. It is well known that depending upon of the parameters and the chosen initial condition the equation (1) can lead either to self-trapping (i.e. local modes or solitons), or to chaos, or to a mixture of the above two behaviours [1], [2], [5]. Instead of (1) we shall consider the equation

$$i\frac{da_n}{dt} + \lambda(a_{n+1} + a_{n-1}) + \mu|a_n|^2 a_n = 0 \tag{2}$$

which is obtained if $a_n \to a_n e^{-i\omega_0 t}$. This equation admits plane wave solutions with constant amplitude

$$a_n = ae^{i(kn-\omega t)}$$

(the lattice constant is taken equal with unity) but with an amplitude depending dispersion relation

$$\omega(k) = -2\lambda\cos k - \mu|a|^2$$

This is a Stokes wave solution and it is well known to be unstable at small modulation of the amplitude (Benjamin-Feir or modulational instability) [6]-[8]. The aim of this note is to study the modulational instability of equation (2) from a statistical point of view, considering a_n as a random variable. In doing this we shall follow the procedure used by several authors to discuss the effects of randomness on the stability of weakly nonlinear waves, especially in hydrodynamics [9], [10].

In the next section a kinetic equation for a two-point correlation function will be obtained. Using a Wigner-Moyal transform the equation is written in a mixed configuration-wave vector space. The linear stability around a homogeneous basic solution is discussed in section 3. An integral stability equation is derived, very similar with the dispersion relation of the linearized Vlasov equation in ionized plasmas. Two forms for the spectrum of the initial unperturbed condition will be considered, namely a Gaussian and a Lorentzian form and in the limit of vanishingly small bands widths the increment of the modulational instability is calculated. Comparison with the continuum limit, when (1) transforms into the nonlinear Schrödinger equation is done. Few concluding remarks are also presented.

2 Kinetic equation for two-point correlation function

Introducing the displacement operator by $a_{n\pm1} = e^{\frac{\partial}{\partial n}} a_n$ the equation (2) becomes

$$i\frac{\partial a_n}{\partial t} + 2\lambda \cosh \frac{\partial}{\partial n} a_n + \mu |a_n|^2 a_n = 0. \tag{3}$$

In order to find a kinetic equation we write (3) for $n = n_1$, multiply it by $a^*_{n_2}$, add it to the complex conjugated of (3) for $n = n_2$ multiplied by a_{n_1} and finally take an ensemble average. One obtains

$$i\frac{\partial}{\partial t} < a_{n_1} a^*_{n_2} > + 2\lambda(\cosh \frac{\partial}{\partial n_1} - \cosh \frac{\partial}{\partial n_2}) < a_{n_1} a^*_{n_2} > +$$
$$\mu(< a_{n_1} a^*_{n_1} a_{n_1} a^*_{n_2} > - < a_{n_2} a^*_{n_2} a_{n_1} a^*_{n_2} >) = 0 \tag{4}$$

which beside the two point correlation function $\rho(n_1, n_2, t) =< a_{n_1}(t) a^*_{n_2}(t) >$ contains also four-point correlation functions. If a_n corresponds to a Gaussian process, and this property is retained during the evolution, a four-point correlation function factorizes exactly in products of two-point correlation functions [11]

$$< a_{n_1} a^*_{n_1} a_{n_1} a^*_{n_2} >= 2 < a_{n_1} a^*_{n_2} >< a_{n_1} a^*_{n_1} >= 2\rho(n_1, n_2)\bar{a^2}(n_1) \tag{5}$$

where $\bar{a^2}(n) =< a_n a^*_n >$ is the ensemble average of the mean square amplitude. Although the factorization (5) is true only for a Gaussian process

we shall assume to be at least approximately valid also for processes slightly different from a Gaussian one, and it represents the main approximation of the present analysis.

It is convenient to use a Wigner-Moyal transform [12]. One introduce the new variables

$$M = \frac{n_1 + n_2}{2}, \qquad m = n_1 - n_2. \tag{6}$$

Then the equation (4) becomes

$$i\frac{\partial\rho}{\partial t} + 4\lambda \sinh\frac{1}{2}\frac{\partial}{\partial M}\sinh\frac{\partial\rho}{\partial m} + 2\mu(\bar{a^2}(M+\frac{m}{2}) - \bar{a^2}(M-\frac{m}{2}))\rho = 0 \tag{7}$$

We consider a chain of N molecules and impose cyclic boundary conditions. The Fourier transform of the two-point correlation function is defined by

$$F(k, M, t) = \sum_m e^{-ikm}\rho(M + \frac{m}{2}, M - \frac{m}{2}, t) \tag{8}$$

where k takes values in the first Brillouin zone (BZ), $k \in (-\pi, \pi)$. The inverse formula is

$$\rho(M+\frac{m}{2}, M-\frac{m}{2}, t) = \frac{1}{M}\sum_k^{BZ} e^{ikm}F(k, M, t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikm}F(k, M, t)dk. \tag{9}$$

For $m = 0$ one obtains

$$\bar{a^2}(N, t) = \frac{1}{N}\sum_k^{BZ} F(k, M, t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} F(k, M, t)dk. \tag{10}$$

Now Fourier transforming equation (7) we get

$$\frac{\partial F}{\partial t} + 4\lambda \sin k \sinh\frac{1}{2}\frac{\partial}{\partial M}F +$$

$$4\mu\sum_{j=1}^{\infty}\frac{(-1)^{j\pm1}}{(2j-1)!2^{2j-1}}\left(\frac{\partial^{2j-1}}{\partial M^{2j-1}}\bar{a^2}(M)\right)\left(\frac{\partial^{2j-1}}{\partial k^{2j-1}}F(k, M)\right) = 0 \tag{11}$$

which is the expected nonlinear evolution equation for $F(k, M, t)$ in a mixed configuration-wave number space (M, k). Using the definition (8) we see that $F(k, M, t)$ is a periodic function in the reciprocal space, $F(k + 2\pi) = F(k)$.

3 Stability analysis

As the unperturbed problem we shall consider a basic solution $F_0(k)$ independent of M and t. This is the random counterpart of the Stokes wave in a deterministic approach. A small perturbation around this homogeneous background is considered, namely

$$F(k, M, t) = F_0(k) + \epsilon F_1(k, M, t) \tag{12}$$

According to (10) we have also

$$\bar{a^2}(M, t) = \bar{a_0^2} + \epsilon \bar{a_1^2}(M, t) \tag{13}$$

where

$$\bar{a_0^2} = \frac{1}{2\pi} \int_{-\pi}^{\pi} F_0(k) dk$$
$$\bar{a_1^2}(M, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} F_1(k, M, t) dk \tag{14}$$

When (12) is introduced into (11), neglecting terms of order ϵ^2, the following linear evolution equation for F_1 is obtained

$$\frac{\partial F_1}{\partial t} + 4\lambda \sin k \sinh \frac{1}{2} \frac{\partial}{\partial M} F +$$
$$4\mu \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{(2j-1)! 2^{2j-1}} \frac{\partial^{2j-1} F_0}{\partial k^{2j-1}} \frac{\partial^{2j-1} \bar{a_1^2}(M)}{\partial M^{2j-1}} = 0 \tag{15}$$

Looking for a plane wave solution

$$F_1(k, M, t) = f_1(k) e^{i(KM - \Omega t)}$$

after little algebra the following stability integral equation is found

$$1 + \frac{\mu}{4\pi\lambda \sin\frac{K}{2}} \int_{-\pi}^{\pi} \frac{F_0(k + \frac{K}{2}) - F_0(k - \frac{K}{2})}{\sin k - \frac{\Omega}{4\lambda \sin\frac{K}{2}}} dk = 0 \tag{16}$$

The modulational instability is related to Ω complex with a positive imaginary part, $Im\Omega > 0$. It is convenient to compare (16) with the similar result for the continuum case of the nonlinear Schrödinger equation [8]

$$1 + \frac{\mu}{K\omega_2} \int_{-\infty}^{\infty} \frac{F_0(k + \frac{K}{2}) - F_0(k - \frac{K}{2})}{k - \frac{\Omega}{2K\omega_2}} dk = 0 \tag{17}$$

Although there are significant differences between the two expressions, when the width of the spectrum $F_0(k)$ is vanishingly small, the final results will look very similar.

3a. Gaussian spectrum

As a first example let us assume $F_0(k)$ to be a Gaussian function

$$F_0(k) = \frac{\sqrt{2\pi}}{\sigma} \bar{a}_0^2 e^{-\frac{k^2}{2\sigma^2}}. \tag{18}$$

This expression doesn't satisfy the periodicity condition but for σ vanishingly small the errors introduced are negligible. Also the relation (14) is satisfied up to exponentially small terms.

It is convenient to introduce the new integration variable $t = \frac{1}{\sqrt{2}\sigma}(k \pm \frac{K}{2})$ and the notations

$$z_\pm = \frac{1}{\sqrt{2}\sigma}\left(\frac{\Omega}{2\lambda \sin K} \pm \tan\frac{K}{2}\right) \tag{19}$$

$$f_\pm(t) = \frac{1}{\sqrt{2}\sigma}\left(\sin\sqrt{2}\sigma t \pm \tan\frac{K}{2}(1 - \cos\sqrt{2}\sigma t)\right).$$

Then (16) becomes

$$\frac{\bar{a}_0^2}{\sqrt{2\pi}\sigma}\ \frac{\mu}{\lambda \sin K} \int_{-\frac{\pi}{\sqrt{2}\sigma}}^{\frac{\pi}{\sqrt{2}\sigma}} e^{-t^2}\left(\frac{1}{z_+ - f_+} - \frac{1}{z_- - f_-}\right) dt = 1. \tag{20}$$

In leading order in σ the integral (20) can be evaluated using the steepest descent method [13]. Denoting $G_\pm(t) = t^2 + ln(z_\pm - f_\pm(t))$, $\quad t_\pm$ the zeros of the first derivatives $\frac{dG_\pm(t)}{dt} = 0$, $\quad A_\pm = \frac{1}{2}\frac{d^2G_\pm}{dt^2}$ for $t = t_\pm$, and extending the integration limits to infinity the integral is given by

$$\sqrt{\pi}\left(\frac{1}{\sqrt{A_+}} e^{-G_+(t_+)} - \frac{1}{\sqrt{A_-}} e^{-G_-(t_-)}\right). \tag{21}$$

In the limit $\sigma \ll 1$ we have approximatively
$t_\pm \simeq \frac{1}{2z_\pm} = \sqrt{\frac{\sigma}{2}}\frac{1}{\frac{\Omega}{2\lambda\sin K} \pm \tan\frac{K}{2}}$, $\qquad e^{-G_\pm(t_\pm)} \simeq \frac{1}{z_\pm}$ and $A_\pm \simeq 1$.
Then the integral becomes

$$\frac{-2\sqrt{2\pi}\sigma \tan\frac{K}{2}}{(\frac{\Omega}{2\lambda \sin K})^2 - (\tan\frac{K}{2})^2}.$$

Considering Ω purely imaginary, $\Omega = i\Omega_i$, we finally get

$$\Omega_i = 4\lambda \sin\frac{K}{2}\sqrt{\bar{a_0^2}\frac{\mu}{\lambda} - \sin^2\frac{K}{2}} \tag{22}$$

and an instability is obtained ($\Omega_i > 0$) if μ and $\lambda > 0$ and if $\sin^2\frac{K}{2} < \bar{a_0^2}\,\frac{\mu}{\lambda}$.

3b. Lorentzian spectrum

A simpler example is a Lorentzian form for $F_0(k)$

$$F_0(k) = \bar{a_0^2}\frac{p\sqrt{1+p^2}}{\sin\frac{K^2}{2} + p^2}. \tag{23}$$

It satisfies the periodicity condition and relation (14). The unperturbed two-point correlation function is easily calculated using (21) in the definition relation (19). Straightforward calculations give

$$\rho_0(m) = \frac{\bar{a_0^2}}{[1 + 2p(\sqrt{1+p^2} + p)]^m} \tag{24}$$

representing an exponentially decreasing law. For $p \ll 1$ we have $\rho_0(m) \simeq \bar{a_0^2}e^{-2pm}$.

In order to calculate the integral (16) it is convenient to introduce the new integration variable $t = \tan\frac{K}{2}$. Then the integral is over the whole real axis and can be done in the t-complex plane. In the new variable $F_0(k \pm \frac{K}{2})$ writes

$$F_0(k \pm \frac{K}{2}) \to \frac{\bar{a_0^2}2p\sqrt{1+p^2}(1+t^2)}{(1+\cos\frac{K}{2} + 2p^2)t^2 \pm 2(\sin\frac{K}{2})t + (1 - \cos\frac{K}{2} + 2p^2)} \tag{25}$$

having poles at

$$t^+_{1,2} = -a \pm ib \qquad t^-_{1,2} = a \pm ib$$

where

$$a = \frac{\sin\frac{K}{2}}{1 + \cos\frac{K}{2} + 2p^2}, \qquad b = \frac{2p\sqrt{1+p^2}}{1 + \cos\frac{K}{2} + 2p^2}. \tag{26}$$

Considering Ω purely imaginary, $\Omega = i\Omega_i$ and denoting $z = \frac{\Omega_i}{4\lambda \sin \frac{K}{2}}$ we have also

$$\frac{1}{\frac{\Omega}{4\lambda \sin \frac{K}{2}} - \sin k} \rightarrow -i\frac{1+t^2}{zt^2 + 2it + z}$$

having poles at

$$t_3 = i\frac{\sqrt{1+z^2}-1}{z} \qquad t_4 = -i\frac{\sqrt{1+z^2}+1}{z}$$

We shall consider z as a small quantity and consequently $t_4 \gg 1$. Closing the contour in the lower complex half-plane t its contribution can be neglected in the first order. Therefore we shall take into account only the poles $t_2^{(\pm)}$ and after straightforward calculations the relation (16) becomes

$$1 = \frac{\mu \bar{a}_0^2}{\lambda \sin \frac{K}{2}} \frac{MA + MX}{X^2 + M^2} \tag{27}$$

where

$$\begin{aligned} A &= 1 + a^2 - b^2, \qquad & B &= 2ab \\ X &= zA + 2b, \qquad & M &= 2a - zB. \end{aligned} \tag{28}$$

When $p \ll 1$ we approximate

$$a \simeq \frac{\sin \frac{K}{2}}{1 + \cos \frac{K}{2}}, \qquad b \simeq \frac{2p}{1 + \cos \frac{K}{2}} \tag{29}$$

terms of order p^2 being neglected. Then (27) can be considerably simplified and finally give us

$$\Omega_i = 4\lambda \sin \frac{K}{2} \left(\sqrt{\frac{\mu}{\lambda}\bar{a}_0^2 - \sin^2 \frac{K}{2}} - 2p\frac{1 + \cos \frac{K}{2} + \cos k}{1 + \cos \frac{K}{2}} \right). \tag{30}$$

Modulational instability occurs for λ and $\mu > 0$, $\sin^2 \frac{K}{2} < \frac{\mu}{\lambda a_0^2}$ and if p is smaller than a critical value. This result is similar with a previous one [16]

obtained with a simplified Lorentzian form for $F_0(k)$. Both results (22) and (30) can be compared with the similar results obtained in the NLS case [8].

$$\begin{aligned}\Omega_i^{(G)} &= 2K\omega_2\sqrt{\frac{\mu}{\omega_1}\bar{a}_0^2 - \frac{K^2}{4}} \\ \Omega_i^{(L)} &= 2K\omega_2\left(\sqrt{\frac{\mu}{\omega_1}\bar{a}_0^2 - \frac{K^2}{4}} - p\right) \qquad (31)\end{aligned}$$

where the superscript G/L refers to Gaussian/Lorentzian form of $F_0(k)$. It is easily seen that (31) are obtained in a long wave limit ($K \ll 1$). In the Lorentzian case both relations (30) and (31) show a behaviour similar with the well known phenomena of Landau damping in plasma physics [14], [15] namely with increasing of p the imaginary part Ω_i can become negative and no instability develops.

In conclusion a complete discrete discussion of the randomness effects on the MI of the self trapping equation was done and the discrete effects are easily seen in the final results, compared with the similar ones found for the NLS equation.

Helpful discussions with Dr. A.S. Cârstea are kindly acknowledged. This research was supported under the contract 66, CERES Program, with the Ministry of Education and Research.

References

[1] J.C. Eilbeck, P.S. Lomdahl, A.C. Scott, Physica D **16**, 318 (1985)

[2] *Davydov's Soliton Revisited. Self Trapping of Vibrational Energy in Proteins*, edited by P.L. Christiansen, A.C. Scott, NATO ASI Series B **243** (Plenum Press, New York, 1990)

[3] A.S. Davydov, N.I. Kislukha, phys.stat.sol.(b) **59**, 465 (1973); **75**, 735 (1976);

A.S. Davydov, Physica Scripta **20**, 387 (1979)

[4] A.S. Davydov, *Solitons in Molecular Systems* (Reidel, Dordrecht, 1985)

[5] L. Cruzeiro-Hansson, H. Feddersen, R. Flesch, P.L. Christiansen, M. Salerno, A.C. Scott, Phys. Rev. B **42**, 522 (1990)

[6] T.B. Benjamin, J.E. Feir, J. Fluid Mech. **27**, 417 (1967)

[7] R.K. Dodd, J.C. Eilbeck, J.D. Gibbon, H.C. Morris, "Solitons and Nonlinear Wave Equations" (Acad. Press, 1982)

[8] D. Grecu, Anca Vişinescu, "Modulational instability in some nonlinear one-dimensional lattices and soliton generation" (to be published in Ann.Univ. Craiova)

[9] I.E. Alber, Proc. Roy. Soc. London A **363**, 525 (1978)

[10] M. Onorato, A. Osborne, M. Serio, R. Fedele, nlin.CD/0202026;

R. Fedele, P.K. Shukla, M. Onorato, D. Anderson, M. Lisak, nlin.CD/0207050

[11] C.M. Gardiner "Handbook of Stochastic Methods" (Springer Verlag, Berlin, 1983)

[12] E. Wigner, Phys. Rev. **40**, 749 (1932)

J.E. Moyal, Proc. Cambridge Phyl. Soc. **45**, 99(1949)

[13] A. Erdelyi, "Asymptotic Expansions" (Dover Publ. 1956);

N.G. Debrujin, "Asymptotic Methods in Analysis" (North Holland Pub., Amsterdam, 1958)

[14] A. Simon, in "Plasma Physics" p. 163 (IAEA, Vienna, 1965);

L.D. Landau, J. Phys. USSR **10**, 25 (1946)

[15] M.J. Ablowitz, H. Segur "Solitons and the Inverse Scattering Transform", see appendix (SIAM, Philadelphia, 1981)

[16] Anca Vişinescu, D. Grecu, "Randomness effects on modulational instability of a discrete self-trapping equation", Proceedings Nat. Conf. Theor. Phys., Bucharest, 2002, in press